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A discrete dislocation dynamics study aiming at understanding fatigue crack initiation

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Abstract

We use discrete dislocation dynamics to build a model for fatigue crack initiation in a surface grain. Dislocations are modeled as line singularities in an elastic medium where they can be generated from pre-existing sources, glide or annihilate. The simulation reveals several features that can potentially give rise to fracture initiation. Three different potential areas of fracture—surface, grain interior and grain boundary—are found which correspond to those found in experiments. Comparison with experimental findings on crack nucleation is hampered by the computational expenses that limit the number of cycles that can be simulated.

Keywords: Dislocation; Fatigue initiation

1. Introduction

Although it is very well documented that fatigue is the reason for the failure of many structures, and although the initiation of the crack is a necessary condition, it is fair to say that fatigue crack initiation still holds many secrets. Extensive experimental studies have revealed that the initiation period of fatigue starts with the accumulation of high densities of dislocations, which may form organized structures. At the free surface of the crystal intrusions and extrusions develop. In many cases protrusions also arise, which often are preferred sites for the nucleation of a fatigue crack. However, crack nucleation has also been seen along grain boundaries [1].

We present here preliminary results of discrete dislocation dynamics simulations that attempt to shed some more light on the nucleation process of a fatigue crack. In this approach, the motion of discrete dislocations within an elastic matrix is used to describe the cyclic plastic deformation inside a surface grain. The simulation accounts for the long-range elastic interactions between dislocations and the free-surface boundary conditions, and is governed by a set of simple constitutive laws.

2. Model

We consider a half-infinite, two-dimensional strip where we imagine that a single grain is located at the free surface so that plastic flow takes place inside this grain but not in the surrounding grains because they are less favorably oriented, see Fig. 1. The rectangular grain has three slip systems at 60° from each other (as a two-dimensional model of an fcc crystal), one being favorably oriented at 45° from the tensile direction. The remote stress, parallel to the free surface, is taken to vary with time in a zig-zag fashion with $\sigma_{\min} = -\sigma_{\max}$.

Plastic flow inside the grain is caused by the motion of a number of discrete dislocations; the surrounding material remains elastic. All dislocations are of edge character with the Burgers vector in the plane of the model. They are treated as singularities in a linear elastic, plane strain, isotropic continuum. Closed-form expressions are used for the long-range displacement and stress fields in the presence of a traction-free surface [2], so that the boundary conditions are directly taken into account. From these singular stress

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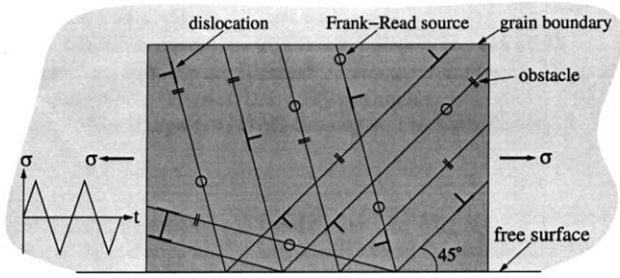

Fig. 1. Plane strain strip of material subjected to a remote cyclic tensile stress parallel to the free surface, with a single grain inside of which discrete dislocation dynamics is adopted.

fields σ_{ij}^J, along with the free surface image stress $\bar{\sigma}_{ij}^I$ [3] and the uniform applied stress $\hat{\sigma}_{ij}$, the Peach–Koehler force on each dislocation I is calculated in each increment according to

$$f^I = n_i^I \left(\sum_{J \neq I} \sigma_{ij}^J + \bar{\sigma}_{ij}^I + \hat{\sigma}_{ij} \right) b_j^I$$

where n_i^I is the normal to the slip plane containing the dislocation I with Burgers vector b_i^I. This force governs the dislocation motion according to the linear drag relation $v^I = f^I/B$ for the dislocation glide velocity, with B the drag coefficient. From the velocity the new dislocation position can be calculated at the end of every time step to update the dislocation structure for the next increment.

In addition, we incorporate the generation of dislocation dipoles from pre-defined two-dimensional Frank–Read sources, when the resolved shear stress exceeds the source strength τ_{nuc} for a sufficiently long time t_{nuc} (see [4] details). Dislocations annihilate when the distance between two dislocations of opposite sign is less than a critical distance which is taken to be 6*b*. Furthermore, dislocations can escape from the crystal at the free surface, leaving behind a step. Finally, dislocations can get pinned at point obstacles. These either represent small precipitates or forest dislocations. The grain boundaries are assumed, for simplicity, to be impenetrable by dislocations, thus representing high angle grain boundaries. The time steps in the incremental procedure are taken small enough (order nanoseconds) that nucleation, pinning and annihilating events are captured.

3. Results and discussion

Results are presented for a 2 μm × 2 μm grain, with the elastic properties being chosen to represent those of aluminum. The grain is dislocation free initially, with dislocation sources (100 μm^{-2}) and obstacles (75 μm^{-2}) randomly distributed over a total of 201 slip planes. The source strengths are randomly chosen from a Gaussian distribution with a mean value of $\tau_{\mathrm{nuc}} = 50$ MPa. All obstacles have a strength of 150 MPa. The peak cyclic stress is taken to be $\sigma_{\max} = 150$ MPa.

During the rising branch of the first cycle, the response of the grain is elastic with the resolved shear stresses on the slip planes increasing linearly. When the resolved shear stress reaches the strength of the weakest dislocation source, a dislocation dipole is generated. Upon further stressing more dislocations get nucleated. During unloading a few dislocations slide back and annihilate. In the compression stage, the dislocation density rises further and subsequently decreases significantly again when unloading from the maximal compressive stress. Nevertheless, after one single cycle there is a net dislocation density. This density accumulates with further cycling, as shown in Fig. 2a.

Fatigue cracks often nucleate inside or near the intersection of a persistent slip band with the surface and follow the primary slip plane. In the model of Fig. 1, the primary slip plane is the one inclined at 45° from the free surface and the applied stress direction. To check for the potential nucleation of a crack, we consider the distribution of the maximal principal tensile stress σ_{I}. Note that each dislocation carries a (1/*r*)-singularity, but that a random dislocation distribution gives just a randomly fluctuating stress field that cannot nucleate fracture, since high stresses have to be present over a sufficiently large region. After 869 and 1897 cycles

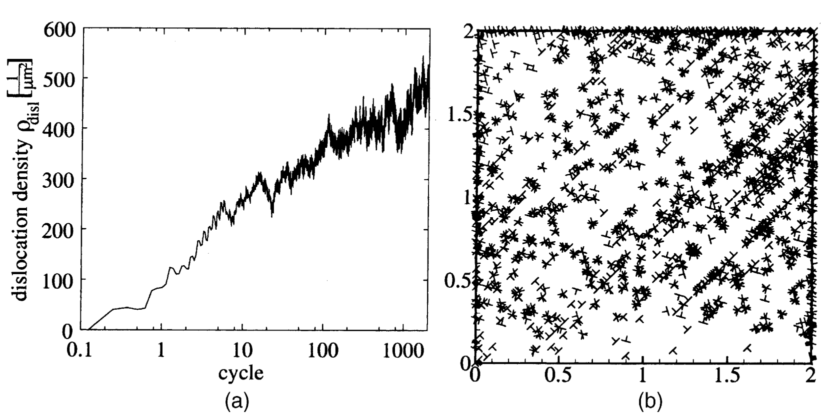

Fig. 2. (a) Dislocation density against the number of cycles (logarithmic scale) in the 2 μm × 2 μm grain. (b) Dislocation distribution after 1897 cycles in the same grain.

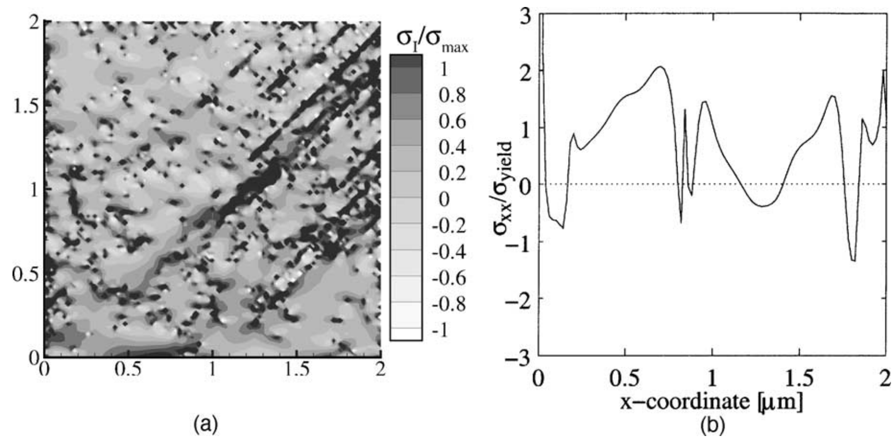

Fig. 3. After 869 cycles: (a) maximum principal stress σ_I normalized by the maximum applied stress in the grain. The free surface is on the bottom side. (b) Profile of σ_{xx} along the free surface normalized by the yield stress.

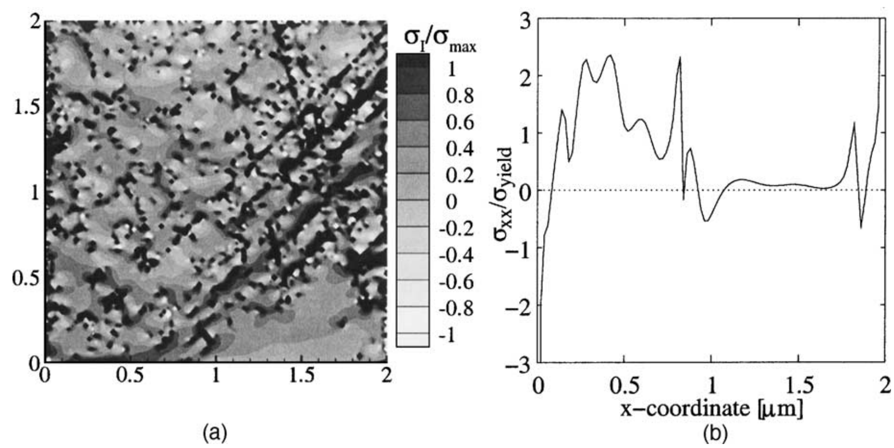

Fig. 4. After 1897 cycles: (a) maximum principal stress σ_I normalized by the maximum applied stress in the grain. The free surface is on the bottom side and the dislocation distribution is shown in Fig. 2b. (b) Profile of σ_{xx} along the free surface normalized by the yield stress.

at zero applied stress, a dislocation distribution has evolved that causes a principal stress field as shown in Fig. 3a and Fig. 4a, respectively.

Inside most of the grain, the stress field is just randomly fluctuating, but there are also extended regions of relatively high tensile stresses near certain parts of the free surface and near the grain boundary. Furthermore, the traces of high-stressed regions inside the grain follow the primary slip system direction. The corresponding principal orientations, which are not shown, are perpendicular to the 45° slip plane and thus point at cracking along the primary slip plane. Comparing the ends of cycle 869 and 1897, one finds an increase in the stress at the grain boundary, and localization of the stress for $x \lesssim 1\,\mu$m along the surface, Figs. 3b and 4b. Most noteworthy after 1897 cycles (Fig. 4a) are the high stresses along the secondary slip direction as well as the widening of the high stressed area along the primary slip planes. At this stage, however, the stresses are of the order of the maximal applied stress, which is too small to cause breaking of inter-atomic bonds.

Crack nucleation is often seen to occur at protrusions. After the simulations have been continued up to 2000 cycles, we indeed start to see protrusions in the simulations [5] of the micrometer size grain as seen experimentally. Subsequently, we traced the variation of the tensile stress parallel to the free surface to see if we could find any indication of a logarithmic singularity, as was suggested by Brown and Ogin [6]. The salient finding in the profiles shown in Figs. 3b and 4b was that indeed there are mostly tensile stress along the free surface causing mode I opening but no sign of a logarithmic singularity. In comparison to cycle 869, the high stresses after 1897 cycles are more localized, but of insufficient intensity to cause cleavage.

4. Concluding remarks

The preliminary results reveal the evolution of dislocation structures, which lead to the accumulation of stresses in the grain and at the grain boundary. The stresses are too low for fracture and the structures are not pronounced enough compared to experiments [7]. This is probably to be attributed to the fact that only a relatively small number of cycles has been simulated.

The model confirms that two distinct fracture mechanisms can occur. As in low-cycle fatigue were mostly transgranular fracture is observed, high stresses are found along traces of the primary slip plane. In high-cycle fatigue, grain boundaries act as sources for fracture leading to intergranular fracture.

Furthermore, the dislocation density increases logarithmically first and gradually seems to saturate, consistent with the experimental finding of large numbers of dislocations in fatigued material. The densities calculated here are about a quarter to one-half of the densities found in experiments. A further increase of dislocation density is expected to occur in later cycles.

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